The Bose-Fermi Kondo model with a singular dissipative spectrum: Exact solutions and their implications

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Quantum dissipation induces a critical destruction of a Kondo screened state, which is of interest in the contexts of quantum critical heavy fermion metals and magnetic nanostructures. The sub-ohmic Bose-Fermi Kondo model provides a setting to study this effect. We find that this many-body problem is exactly solvable when the spectrum of the dissipative bosonic bath, $J(\omega)$, is singular, corresponding to $J(\tau) = \text{const.}$. We determine the local spin correlation functions, showing that the singular *longitudinal* fluctuations of the bosonic bath dominate over the transverse ones. Our results provide evidence that the local quantum critical solution, derived within the extended dynamical mean field approach to the Kondo lattice model, has a zero residual entropy.

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The Bose-Fermi Kondo model (BFKM)[1, 2] has become of considerable interest in a number of different contexts, including the extended dynamical mean field approach to the heavy fermion quantum criticality[3] and the dissipative effects in mesoscopic structures[4, 5]. The model describes a quantum impurity spin coupled simultaneously to a conduction-electron bath[6] and to a dissipative bosonic continuum[7, 8]. The coupling of the local moment to conduction electrons leads to the Kondo screening effect. The coupling to the bosonic bath, on the other hand, causes the critical suppression of the Kondo effect. The latter is the key ingredient of the local quantum critical solution to the Kondo lattice model[3], and has received some fairly direct support from the experiments in heavy fermions[9, 10]. In even broader contexts, models such as BFKM serve as prototype systems to study quantum dissipation and quantum coherence[7].

The BFKM has a rich phase diagram, which is sensitive to the form of the spectral density of the bosonic bath:

$$J(\omega) \propto |\omega|^{1-\epsilon}\,\mathrm{sgn}(\omega)\ . \tag{1}$$

Most of the previous studies have focused on the sub-ohmic case with $0 < \epsilon < 1$. The perturbative renormalization group (RG) analysis[1, 2, 11, 12] shows that spin-anisotropy is a relevant perturbation, and indeed the Kondo-destroyed phase of the Ising-anisotropic BFKM[1, 11, 13, 14, 15, 16] differs qualitatively from that of the spin-isotropic BFKM[17, 18]. The cases of singular bosonic spectrum [$J(\omega)$ being divergent in the zero-frequency limit], $\epsilon > 1$, have received much less attention. (A singular bosonic spectrum might be realizable in some low dimensional ferromagnetic single-electron structures[5].) One may argue [19] on general grounds that the large bosonic spectral weight at low energies implies that an infinitesimal coupling between the local moment and the bosonic bath will suppress the Kondo effect. For the Ising-anisotropic BFKM, the numerical renormalization group (NRG) work of Glossop and Ingersent [16] has indeed demonstrated this.

Several factors have motivated us to search for an exact solution to BFKM. It will put the above perturbative, numerical, or saddle-point results on a more firm ground, thereby elucidating the physics of not only the Kondo destruction but also the quantum dissipation/coherence in general. In addition, it may help resolve some apparent inconsistency concerning the entropy of the local quantum critical solution to the Kondo lattice system. Some general considerations suggest a zero residual entropy (see below), yet Kircan and Vojta [20] have interpreted their results for a dynamical large-N limit of the spin-isotropic BFKM as signaling a contrary conclusion.

In this letter, we show that the BFKM with a singular bosonic bath, corresponding to $\epsilon = 2$, is exactly solvable. The exact solution establishes that an infinitesimal coupling between the local moment and the bosonic bath indeed causes a Kondo destruction. Surprisingly, we find that the spin-isotropic problem has the same universal properties as the Ising-anisotropic one, which implies that the longitudinal dissipative coupling plays a dominant role. This effect turns out to be missed by the large-N limit of Ref. [20] in an interesting way.

The Hamiltonian for the BFKM is

$$H = H_F + H_B + H_J + H_g + H_h. \tag{2}$$

Here, $H_F = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma}$ and $H_B = \sum_{p,a} w_p \Phi^\dagger_{pa}\Phi_{pa}$ respectively describe a conduction-electron band and a bosonic bath, and ε_k and w_p their corresponding dispersions. $H_J = (J_\perp/2)[s^-_c(0)S^+ + s^+_c(0)S^-] + J_{||} s^z_c(0) S^z$ specifies the Kondo coupling between a spin-1/2 local moment, $\vec{S}$, and the conduction electron spin $\vec{s}_c = \sum \frac{1}{2} c^\dagger_{k\sigma} \vec{\tau}_{\sigma,\sigma'} c_{k\sigma'}$ (with $\vec{\tau}$ being the Pauli matrices) and $H_g = \sum_{a=1}^{3} g_a \Phi^a S^a$ the impurity coupling to the bosonic field, with $\Phi^a \equiv \sum_p (\Phi_{pa} + \Phi^\dagger_{-pa})$ at the impurity site 0. The dissipative bosonic spectrum, $J(\omega) \equiv \sum_p [\delta(\omega - w_p) - \delta(\omega + w_p)]$, is taken to have the form of Eq. (1).

In order to probe the local spin responses, introduces a local magnetic field, h, via $H_h = hS^z$.

The partition function can be written in the path-integral form. The quantum impurity spin $\vec{S}$ is represented by an $SU(2)$ coherent state $S\vec{\Omega}(\tau)$ with the constraint $\vec{\Omega}^2(\tau) = 1$. A Berry phase term $\mathcal{S}_B[\vec{\Omega}]$ characterizes the quantum dynamics of the impurity spin. Meanwhile, the bosonic bath can be traced out, leading to a long-ranged interaction (along the τ-dimension) for the impurity spin[1, 2]:

$$Tr \exp\{-\beta(H_B + H_g)\} = Z_b \int \mathcal{D}\vec{\Omega} \exp\{-i\mathcal{S}_B[\vec{\Omega}]\} \quad (3)$$
$$\times \exp\{\sum_{a=1}^{3} \int_0^\beta \int_0^\beta d\tau_1 d\tau_2 \frac{g_a^2 S\Omega^a(\tau_1) S\Omega^a(\tau_2)}{4|\tau_2 - \tau_1|^{2-\epsilon}}\},$$

with Z_b being the partition function of the bosonic bath. (Note that the purely classical model defined along a chain, $0 < \tau < \beta$, is considered to be ill-defined for $1 < \epsilon \leq 2$, since the long-ranged interaction makes the ground state energy per unit length diverge in the $\beta \to \infty$ limit, but the quantum problem we consider is still well-defined.[21]) For $\epsilon = 2$, the long-range interaction in the last term becomes $\sum_{a=1}^{3} [\int_0^\beta d\tau g_a S\Omega^a(\tau)/2]^2$, which can be further decomposed by introducing a Hubbard-Stratanovich vector $\vec{\lambda} = (\lambda_1, \lambda_2, \lambda_3)$:

$$\exp\{\sum_{a=1}^{3} [\int_0^\beta d\tau S g_a \Omega^a(\tau)/2]^2\} =$$
$$\pi^{-3/2} \int d\vec{\lambda} \exp\{-\vec{\lambda}^2 - \sum_{a=1}^{3} g_a \lambda_a \int_0^\beta d\tau S\Omega^a(\tau)\}. \quad (4)$$

The total partition function of the BFKM, when rewritten in the operator formalism, becomes

$$Z = \mathrm{Tr} e^{-\beta H} = \pi^{-3/2} Z_b \int d\vec{\lambda} e^{-\vec{\lambda}^2} \mathrm{Tr} e^{-\beta \tilde{H}(\vec{\lambda})},$$
$$\tilde{H}(\vec{\lambda}) = H_F + H_J + H_h + H_{\vec{\lambda}}, \quad (5)$$

where $H_{\vec{\lambda}} = \sum_{a=1}^{3} g_a \lambda_a S^a$. Hence, we are led to solve the BFKM, Eq. (2), in terms of a pure Fermi-Kondo model in the presence of a Gaussian-distributed magnetic field $\vec{\lambda}$, along with the external field h.

The Bose-Kondo model. We first consider the case with $g_a = g$ (for $a = 1, 2, 3$) and in the absence of conduction electrons, *i.e.*, the $SU(2)$ Bose-Kondo model. Here, $\tilde{H}(\vec{\lambda}) = hS^z + g\vec{\lambda} \cdot \vec{S}$. Using the parameterization $\vec{\lambda} = (\lambda \sin\varphi \cos\theta, \lambda \sin\varphi \sin\theta, \lambda \cos\varphi)$, we can specify the eigenvalues of $\tilde{H}(\vec{\lambda})$ as $\pm g\tilde{\lambda}/2$, with $\tilde{\lambda} = \lambda\sqrt{(1-y)^2 + 4y\cos^2\frac{\varphi}{2}}$ and $y = \frac{h}{g\lambda}$. Inserting these into Eq. (5) leads to the impurity partition function, $Z_{loc} = Z_b^{-1} Z$:

$$Z_{loc} = \left(2\cosh\frac{h\beta}{2} + \frac{g^2\beta}{2} \frac{\sinh\frac{h\beta}{2}}{h}\right) e^{\frac{g^2\beta^2}{16}}. \quad (6)$$

It follows that the static local spin susceptibility is

$$\chi_{loc} = \frac{1}{\beta} \frac{\partial^2 \ln Z_{loc}}{\partial h^2}|_{h=0} = \frac{\beta}{12} \frac{3 + g^2\beta^2/8}{1 + g^2\beta^2/8} \xrightarrow{\beta\to\infty} \frac{\beta}{12} \quad (7)$$

The asymptotic behavior in the low-temperature limit has a Curie form, $\chi_{loc}(T \to 0) = \beta/12$, with a reduced Curie constant (1/12 instead of the free-spin value, 1/4).

The dynamical local spin-spin correlation function, $\chi_{loc}(\tau) \equiv \langle S^z(\tau) S^z(0)\rangle_{loc}$, is obtained from a Gaussian averaging: $\chi_{loc}(\tau) = \left(\pi^{-3/2}/Z_{loc}\right) \int d\vec{\lambda} e^{-\vec{\lambda}^2} A(\lambda)$, where $A(\lambda) = Tr e^{-\beta \tilde{H}[\vec{\lambda}]} S^z(\tau) S^z(0)$. The trace amounts to $\sum_{n,m} e^{-E_n\beta} e^{(E_n - E_m)\tau} |\langle n|S^z|m\rangle|^2$, where n and m run over all the eigenstates of $\tilde{H}[\vec{\lambda}]$: $|+\rangle = (\cos\frac{\varphi}{2} e^{-i\frac{\theta}{2}}, \sin\frac{\varphi}{2} e^{i\frac{\theta}{2}})$, $|-\rangle = (-\sin\frac{\varphi}{2} e^{-i\frac{\theta}{2}}, \cos\frac{\varphi}{2} e^{i\frac{\theta}{2}})$. It follows that $A(\lambda) = \frac{1}{2}[\cos^2\varphi \cosh\frac{g\lambda\beta}{2} + \sin^2\varphi \cosh\frac{g\lambda(\beta - 2\tau)}{2}]$ and, in turn,

$$\chi_{loc}(\tau) = \frac{1}{12}[1 + \frac{2 + \frac{g^2(\beta-2\tau)^2}{4}}{1 + \frac{g^2\beta^2}{8}} e^{-\frac{g^2}{4}\tau(\beta-\tau)}] \underset{\beta\to\infty}{\xrightarrow{\tau\to\beta/2}} \frac{1}{12}. (8)$$

In the asymptotic low-temperature and long-time limit ($\tau \to \beta/2$, $\beta \to \infty$), it also has a Curie form. The full result is also illustrated in Fig. 1.

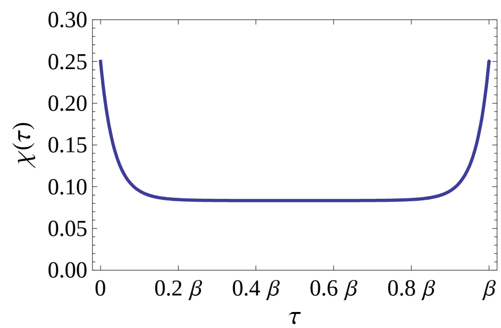

FIG. 1: The dynamical locl spin susceptibility of the $SU(2)$ Bose-only Kondo model at $\epsilon = 2$ (with $g = 1$ and $\beta = 10$).

We next consider the Ising case, *i.e.*, $g_1 = g_2 = 0, g_3 = g$. The impurity partition function is now

$$Z_{loc} = 2\cosh\frac{h\beta}{2} e^{\frac{g^2\beta^2}{16}}. \quad (9)$$

Both the static and dynamical local spin susceptibility have simple Curie forms: $\chi_{loc} = \beta/4$, and $\chi_{loc}(\tau) = 1/4$.

To summarize, the local spin response of both the $SU(2)$ and the Ising cases has a Curie form in the low temperature limit. For the $SU(2)$ problem, the fact that it has the same universal behavior as the Ising case implies that it too is controlled by the $g^* = \infty$ fixed point; in other words, the longitudinal fluctuations dominate over the transverse ones. This is in contrast to the $\epsilon < 1$ case, where the $SU(2)$ and Ising problems are controlled

by a finite-g^* fixed point and a $g^* = \infty$ one, respectively. [1, 2, 11, 12] Our exact result for the $\epsilon = 2$ case reveals the link between a singular bosonic spectrum and dominant longitudinal fluctuations. We therefore expect that, for the $1 < \epsilon < 2$ cases too, the $SU(2)$ problem will be controlled by the fixed point at $g^* = \infty$.

The Bose-Fermi Kondo model. We now incorporate the Kondo coupling as well. The spin-isotropic case requires the usage of Bethe-ansatz method, which will be discussed elsewhere[22]. Here we consider the case in which the pure fermionic Kondo part is placed at its Toulouse point[6] and, moreover, the impurity-boson coupling is purely Ising. Since the spin-anisotropy in the impurity-bosonic coupling is irrelevant and our results will demonstrate that an infinitesimal coupling to the bosonic bath leads to the Kondo destruction, the spin-isotropic BFKM should behave similarly.

When the Kondo couplings take the Toulouse values, the model Eq. (5) can be mapped[6] to the following non-interacting spinless resonant level model (RLM): $H_T(\lambda) = \sum_{\vec{k}} \left[\varepsilon_{\vec{k}} c^\dagger_{\vec{k}} c_{\vec{k}} + V(c^\dagger_{\vec{k}} d + h.c.)\right] + \varepsilon_d(d^\dagger d - \frac{1}{2})$. Here, the impurity spin is represented by $S^z \to d^\dagger d - 1/2$, $S^+ \to d^\dagger$, and $S^- \to d$, with d describing a spinless fermion. The hybridization V is proportional to $J_\perp$, while $\varepsilon_d = g\lambda + h$. After integrating out the fermionic bath, we obtain $Z_T = \pi^{-1/2} \int d\lambda e^{-\lambda^2} \mathrm{Tr} e^{-\beta H_T(\lambda)} = Z_c Z_{loc}$. Here, Z_c is the partition function of the electron bath, and $Z_{loc} = \pi^{-1/2} \int d\lambda e^{-\lambda^2} Z_{loc}[\lambda]$ with

$$Z_{loc}[\lambda] = \; 2\exp\{-\beta \int_{-D}^{D} \frac{d\omega}{\pi} n(\omega) \arctan\frac{\Gamma}{\omega - \epsilon_d}\} \cdot \cosh(\frac{\beta\epsilon_d}{2}), \tag{9}$$

where $n(\omega) = [1 + \exp(\beta\omega)]^{-1}$ is the Fermi function, $\Gamma = \pi\rho_0 V^2$ the bare resonance width, and ρ_0 the conduction-electron density of states at the Fermi energy. Without loss of generality, we assume a flat band for the electrons, taking the usual limit of a large bandwidth D ($\gg \Gamma$).

Eq. (9) has been derived with care, containing not only the usual phase shift contribution [6], but also a residual atomic term. Indeed, it recovers the results for both the Ising bosonic Kondo model ($\Gamma = 0$) and the conventional RLM ($g = 0$). When both couplings Γ and g are non-zero, the Gaussian averaging over λ complicates the problem. We focus on the zero-field static local susceptibility. It is straightforward to show that

$$\chi_{loc} = \frac{\int_{-\infty}^{\infty} d\lambda e^{-\lambda^2} \chi_{loc}[\lambda] Z_{loc}[\lambda]}{\int_{-\infty}^{\infty} d\lambda e^{-\lambda^2} Z_{loc}[\lambda]} |_{h=0}, \tag{10}$$

where $\chi_{loc}[\lambda] = \{\frac{\partial}{\partial h} M_{loc}[\lambda] + \beta M^2_{loc}[\lambda]\}$ and $M_{loc}[\lambda] = \frac{1}{\beta} \frac{\partial \ln Z_{loc}[\lambda]}{\partial h}$. At low temperatures, we use the asymptotic approximation $n(\omega) \approx \Theta(-\omega)$ (Sommerfeld expansion, valid up to corrections of order of T^2/Γ) and integrate over ω, obtaining $\chi_{loc}[\lambda] = \frac{1}{\pi\Gamma} \frac{\Gamma^2}{\Gamma^2 + g^2\lambda^2} + \frac{\beta}{\pi^2} \arctan^2 \frac{g\lambda}{\Gamma}$ and $Z_{loc}[\lambda] = \exp\{\frac{\beta g \lambda}{\pi} \arctan\frac{g\lambda}{\Gamma} - \frac{\beta\Gamma}{2\pi} \ln[1 + (\frac{g\lambda}{\Gamma})^2]\} Z'$, where Z' is independent of λ in the limit $D/\Gamma \to \infty$.

In the weak boson-impurity coupling regime, $g/\Gamma \ll 1$, the λ-integrals in Eq.(10) can be asymptotically approximated by introducing a cut-off $\Lambda \approx \Gamma/g \gg 1$. Within the cut-off ($|\lambda| \ll \Lambda$, called region I below), the dummy variable $\frac{g\lambda}{\Gamma}$ is always small such that expansions like $\arctan\frac{g\lambda}{\Gamma} \approx \frac{g\lambda}{\Gamma}$ are appropriate. Outside the cut-off ($|\lambda| \gg \Lambda$, region II), $\frac{g\lambda}{\Gamma}$ is large enough and one has $\arctan\frac{g\lambda}{\Gamma} \approx \mathrm{sgn}(\lambda)\frac{\pi}{2}$. $\chi_{loc}[\lambda]$ then becomes $\frac{1}{\pi\Gamma} + \frac{\beta}{\pi^2}\left(\frac{g\lambda}{\Gamma}\right)^2$ and $\frac{\beta}{4}$ for $|\lambda| \ll \Lambda$ and $|\lambda| \gg \Lambda$, respectively. $Z_{loc}[\lambda]$ contains a dimensionless combination, $\alpha = \frac{\beta g^2}{2\pi\Gamma}$. A characteristic temperature scale, $T^* = \frac{g^2}{2\pi\Gamma}$ (corresponding to $\alpha = 1$), arises, separating two limiting temperature regimes with distinct asymptotic behavior for χ_{loc}. In the low temperature regime, *i.e.*, $T \ll T^*$ (or $\alpha \gg 1$), the λ-integration is dominated by the region-II contribution, and $\chi_{loc} \approx \frac{\beta}{4}$. In the higher temperature regime, $T^* \ll T \ll \Gamma$ (or $\alpha \to 0$), on the other hand, the region-I contribution dominates, and $\chi_{loc} \approx \frac{1}{\pi\Gamma}$. A smooth, but broad, crossover takes place around $T \sim T^*$. The phase diagram is illustrated in Fig. 2.

In short, for a fixed non-zero Kondo coupling (and, hence, non-zero Γ), the local spin susceptibility in the low-temperature limit turns to a Curie form for any non-zero g. This implies that an infinitesimal g causes a destruction of the Kondo effect; the BFKM is controlled by the fixed point associated with the Bose-only Kondo model solved in the previous section.

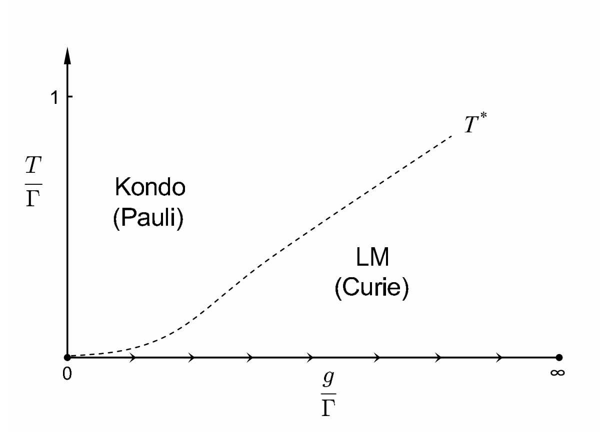

FIG. 2: The phase diagram of the present BFKM. χ_{loc} has the Curie or Pauli forms when $T \ll T^*$ or $T^* \ll T \ll \Gamma$; for $g \ll \Gamma$, $T^* \approx g^2/(2\pi\Gamma)$.

Implications for the EDMFT solution of the Kondo lattice model. The extended dynamical mean field approach to the Kondo lattice model is studied through a BFKM with self-consistent spectra for the bosonic and fermionic baths. In the local quantum critical

solution,[3, 13, 23, 24] the self-consistent bosonic bath has a spectrum with $\epsilon = 1^-$.

For $\epsilon < 1$, we have the standard sub-ohmic situation in which an unstable fixed point (critical, referred to as "C") separates the Kondo and LM fixed points.[11, 12] NRG studies of the Ising-anisotropic BFKM[16] found that, for $1 < \epsilon < 2$, an infinitesimal g leads to Kondo destruction. (Similar results were inferred from an O(N) representation of the Ising-anisotropic BFKM[19].) In other words, at ϵ exactly equals to 1, "C" and the Kondo fixed points are merged and the impurity entropy will vanish. We expect the impurity entropy to be a smooth function of ϵ (which is consistent with the NRG result[25]), so the impurity entropy should vanish at $\epsilon = 1^-$ as well. It follows that the corresponding solution to the Kondo lattice has a vanishing residual entropy, which has been experimentally seen in $YbRh_2Si_2$, a prototype quantum critical heavy fermion metal.[26].

The situation is very different in the large-N limit discussed in Ref. [20], where "C" and the Kondo fixed points are still separated even for $1 < \epsilon < 2$.[27] Moreover, the impurity entropy, at both the "C" and the LM fixed points, are finite for the entire range of $0 < \epsilon < 2$, including at $\epsilon = 1$.

Our exact results imply that the large-N limit becomes problematic when the bosonic bath is singular. The local susceptibilities of both the LM and "C" fixed points of the large-N limit were shown to have $\chi_{loc}(\tau) \sim 1/\tau^{\eta}$, with $\eta = \epsilon$ for the entire range of $0 < \epsilon \leq 2$ [20]; the structure of fixed points remains the same over this range $0 < \epsilon \leq 2$ [20]. This would give rise to $\eta = 2$ for $\epsilon = 2$. But our exact solution for the $SU(2)$ case [*cf.*, Eq. (8) and Fig. 1] shows that $\eta = 0$ for $\epsilon = 2$. The problem lies in the large-N-limit's under-estimation of the longitudinal fluctuations, which is of order $1/N$. As we discussed earlier, when the bosonic bath has a singular spectrum ($\epsilon > 1$) and for any finite-N, the strong longitudinal fluctuations dominates over the transverse fluctuations, and the spin-isotropic problem fall in the same universality class as the Ising case. This implies that the structure of the fixed points of the spin-isotropic BFKM changes as ϵ passes through 1.

Keeping track of the longitudinal fluctuations is also important to enforce the Griffiths' bound[28], which requires $\chi_{loc}(\tau)$ *not* to decay faster than the interaction, $1/\tau^{2-\epsilon}$. This bound is violated (for $\epsilon > 1$) by the $N = \infty$ result,[20] $\chi_{loc}(\tau) \sim 1/\tau^{\epsilon}$. A contribution of order $1/\tau^{2-\epsilon}$ to $\chi_{loc}(\tau)$ occurs at order $1/N$, which is missed in the $N = \infty$ limit. On the other hand, our exact result for the $SU(2)$ problem at $\epsilon = 2$, $\chi_{loc}(\tau) \sim 1/\tau^0$, satisfies the Griffiths' bound.

In conclusion, we have presented the first exact solution to the Bose-Fermi Kondo model. Our results display the physics of dissipation-induced Kondo destruction, an effect that is of extensive current interest in the understanding of quantum criticality in heavy fermion metals. Our results also establish the important role that the longitudinal fluctuations of the dissipative bath plays in the Kondo destruction, which has been missed in an interesting way in a large-N formulation of this problem. The new understandings achieved here have allowed us to elucidate the issue of zero residual entropy of the local quantum critical solution to the Kondo lattice models.

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